Supplementary Information

Influence of the alkenyl structures on the epoxidation of unsaturated fatty acid methyl esters and vegetable oils

Supplementary figures

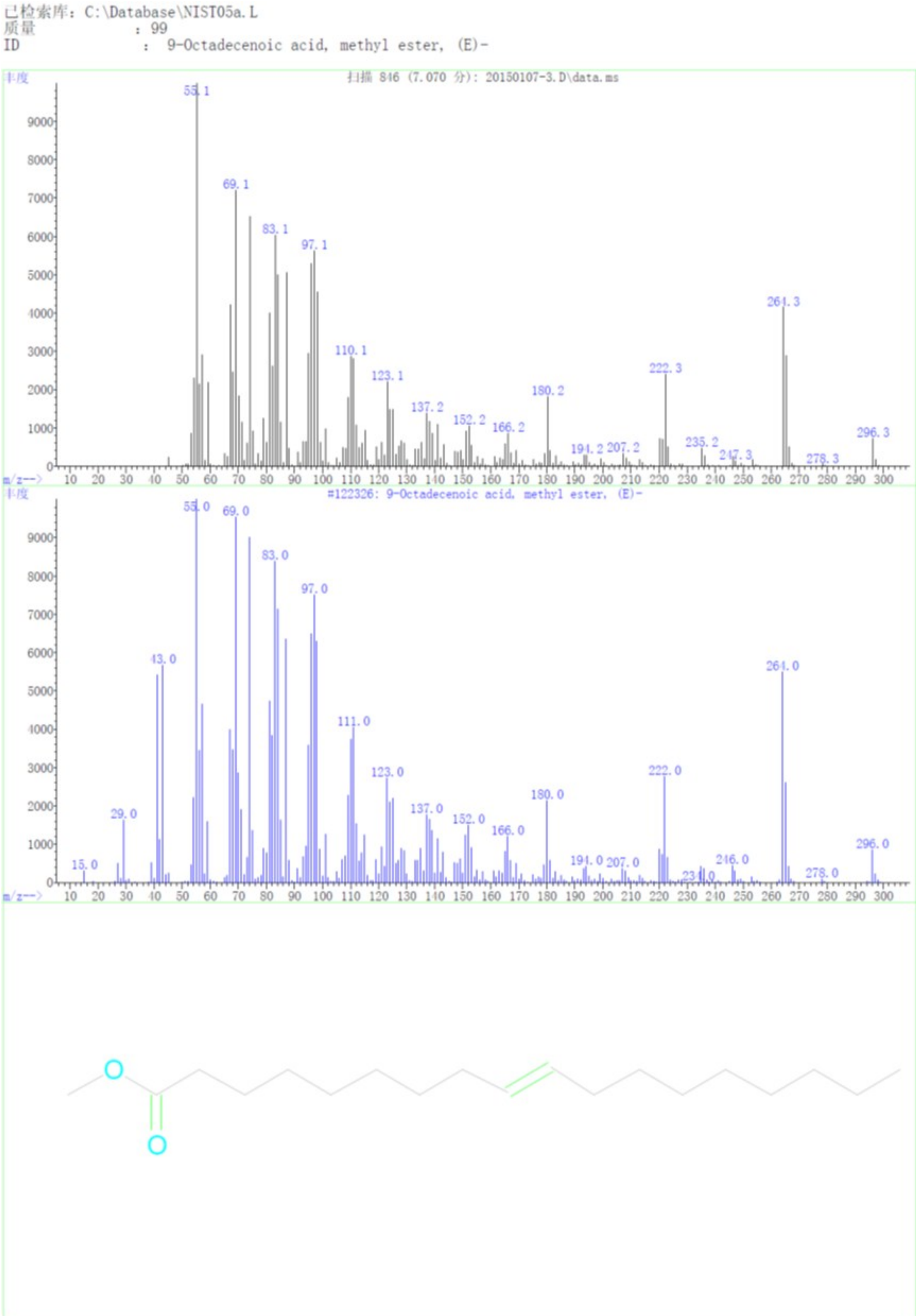


Fig. S1 GC-MS results of 1 in the trace of the epoxidation of methyl oleate

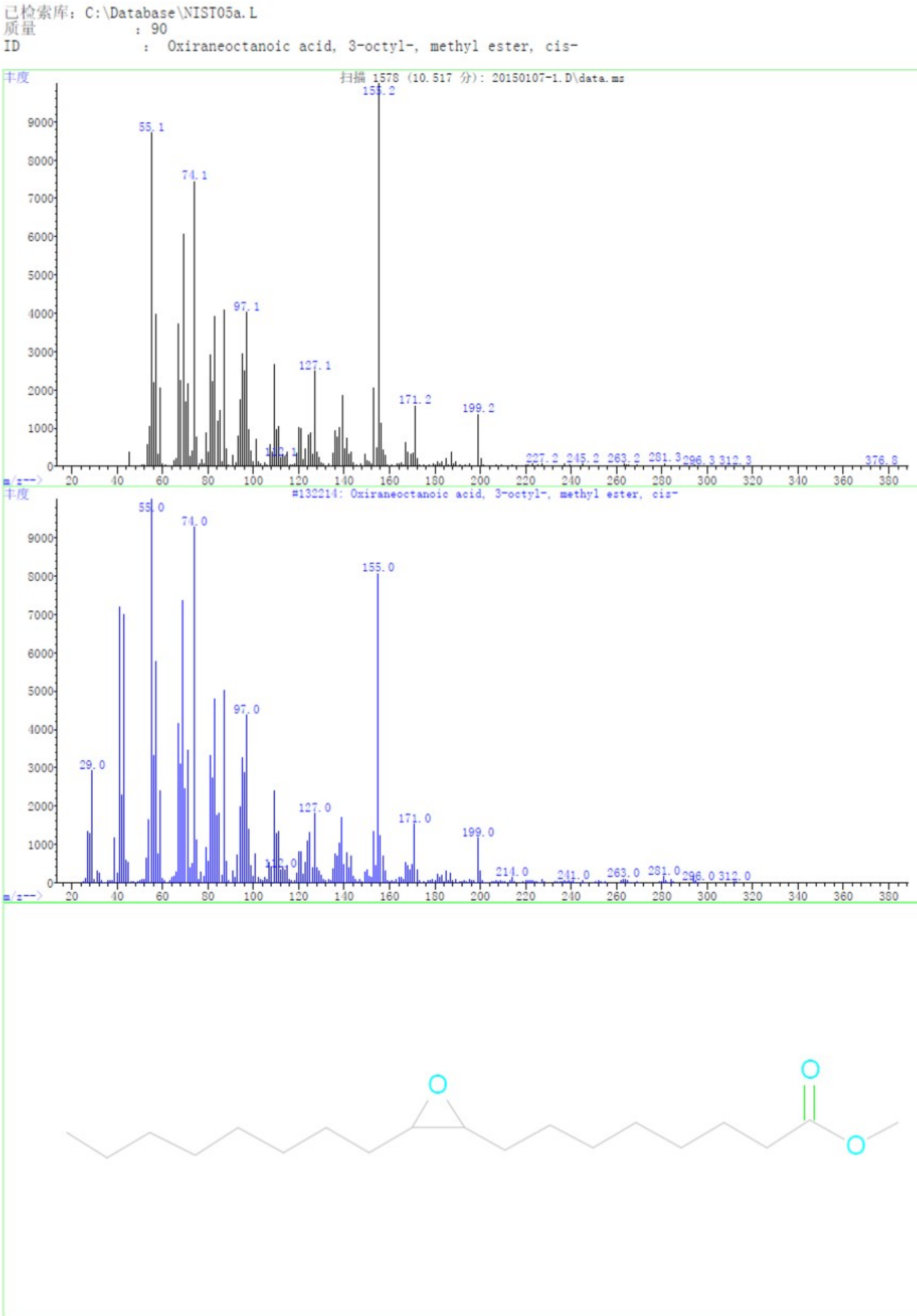


Fig. S2 GC-MS results of 2 in the trace of the epoxidation of methyl oleate

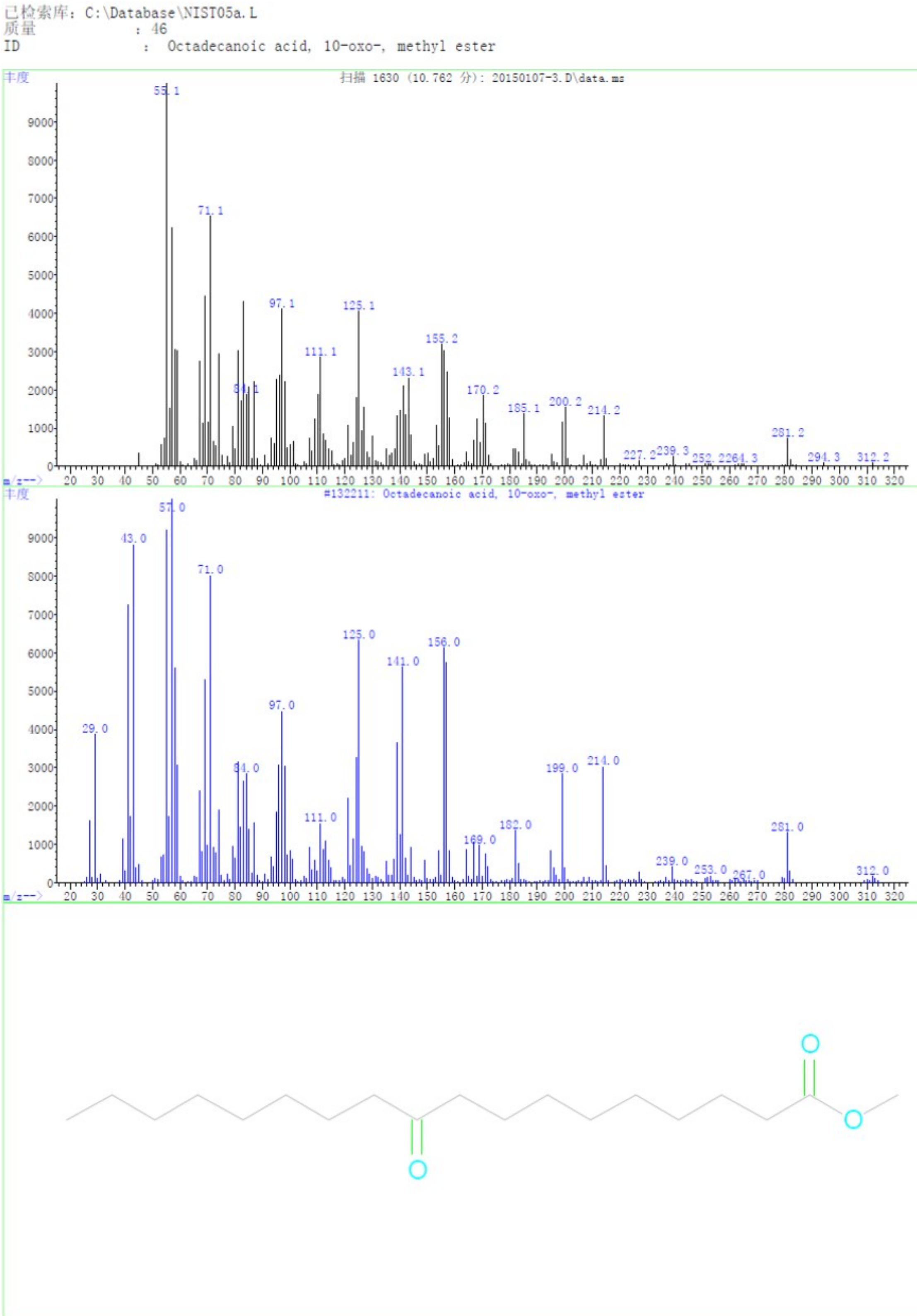


Fig. S3 GC-MS results of 3 for the epoxidation of methyl oleate

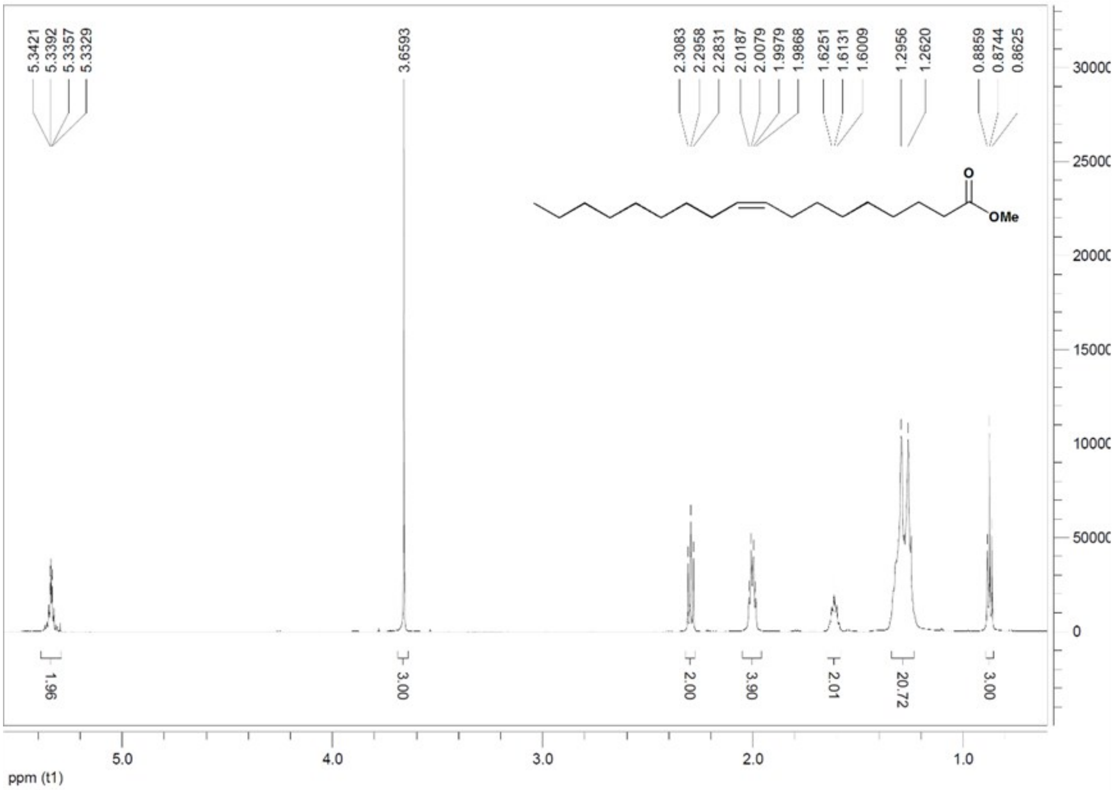


Fig. S4 ^{1}H-NMR spectra of 1 for the epoxidation of methyl oleate

^{1}H-NMR (600MHz, $CDCl_3$): δ (ppm) = 5.34(m, -CH=CH-), 3.66(s, $-OCH_3$), 2.30(t, *J*=7.56Hz, $-CH_2$-CO-), 2.02(m, $-CH_2$-CH=CH-CH_2-), 1.62(t, *J*=7.26Hz, $-CH_2$-CH_3), 1.29(m, $-(CH_2)_n-$) and 0.87(t, *J*=7.02Hz, $-CH_3$).

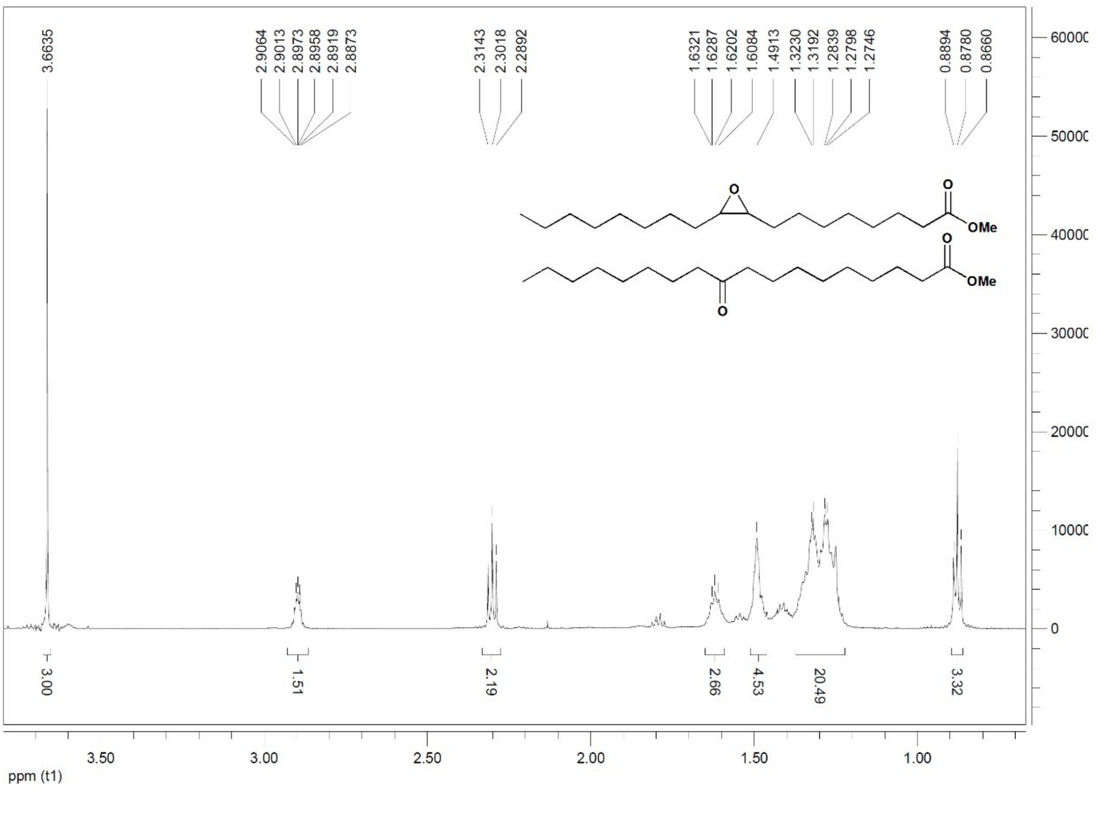


Fig. S5 ^{1}H-NMR spectra of 2 from epoxidation of methyl oleate

^{1}H-NMR (600MHz, $CDCl_3$): δ (ppm) = 3.66(s, $-OCH_3$), 2.89(m, -CHOCH-/$-CH_2$-CO-CH_2-), 2.30(t, *J*=7.53Hz, $-CH_2$-CO-), 1.49(m, $-CH_2$-CH=CH-CH_2-), 1.62(m, $-CH_2$-CH_3), 1.29(m, $-(CH_2)_n$-) and 0.87(t, *J*=7.02Hz, $-CH_3$).

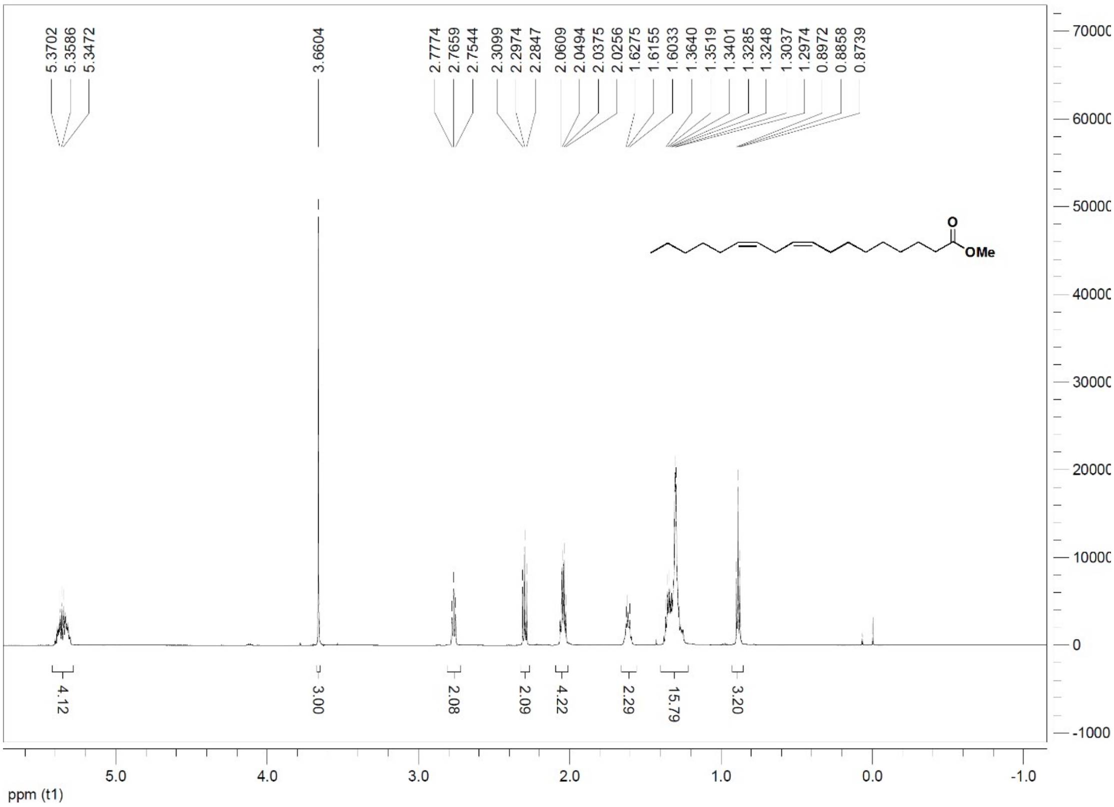


Fig. S6 ^{1}H-NMR spectra of 4 for the epoxidation of methyl linoleate

^{1}H-NMR (600MHz, $CDCl_3$): δ (ppm) = 5.35(m, -CH=CH-), 3.66(s, $-OCH_3$), 2.76(t, *J*=6.90.Hz, -CH=CH-CH_2-CH=CH-), 2.30(t, *J*=7.56Hz, $-CH_2$-CO-), 2.07(m, $-CH_2$-CH=CH-CH_2-CH=CH-CH_2-) 1.62(t, *J*=7.26Hz, $-CH_2$-CH_3), 1.30(m, $-(CH_2)_n$-) and 0.87(t, *J*=6.99Hz, $-CH_3$).

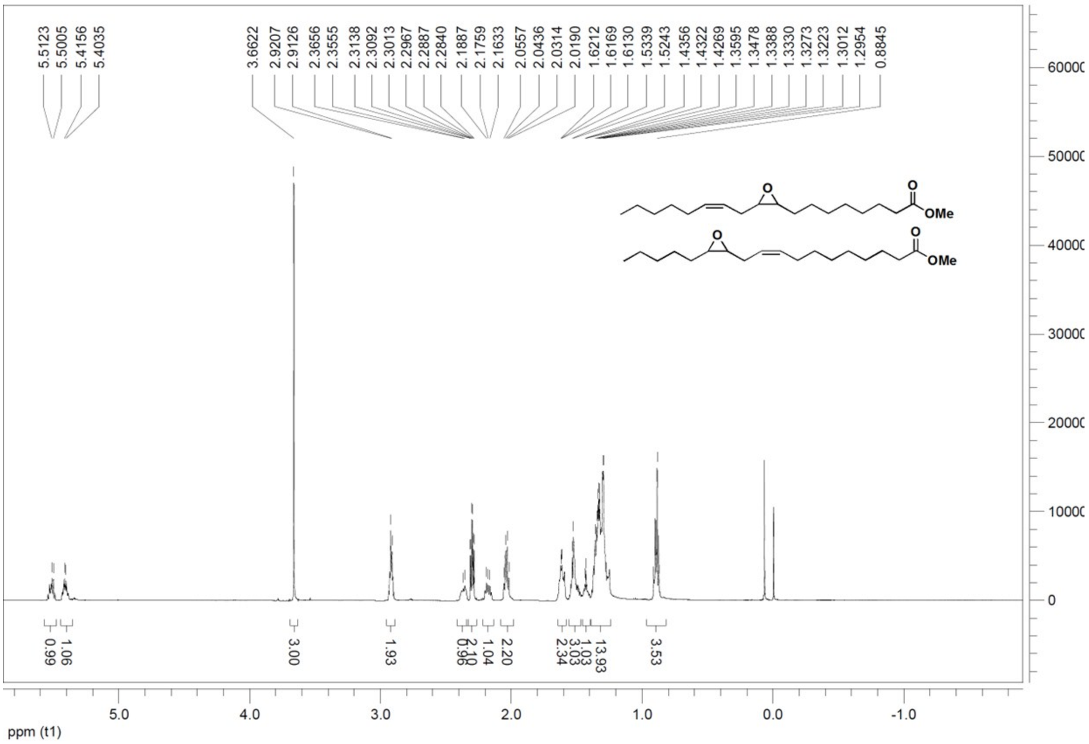


Fig. S7 ^{1}H-NMR spectra of 5 for the epoxidation of methyl linoleate

^{1}H-NMR (600MHz, $CDCl_3$): δ (ppm) = 5.40(m, -CH=CH-), 3.66(s, $-OCH_3$), 2.91(m, -CH-O-CH-), 2.35(m, $-CH_2$-CH-O-CH-), 2.29(m, $-CH_2$-CO-), 2.05(m, $-CH_2$-CH=CH-CH_2-CH-O-CH-CH_2-), 1.61(m, $-CH_2-CH_3$), 1.30(m, $-(CH_2)_n-$) and 0.87(m, $-CH_3$).

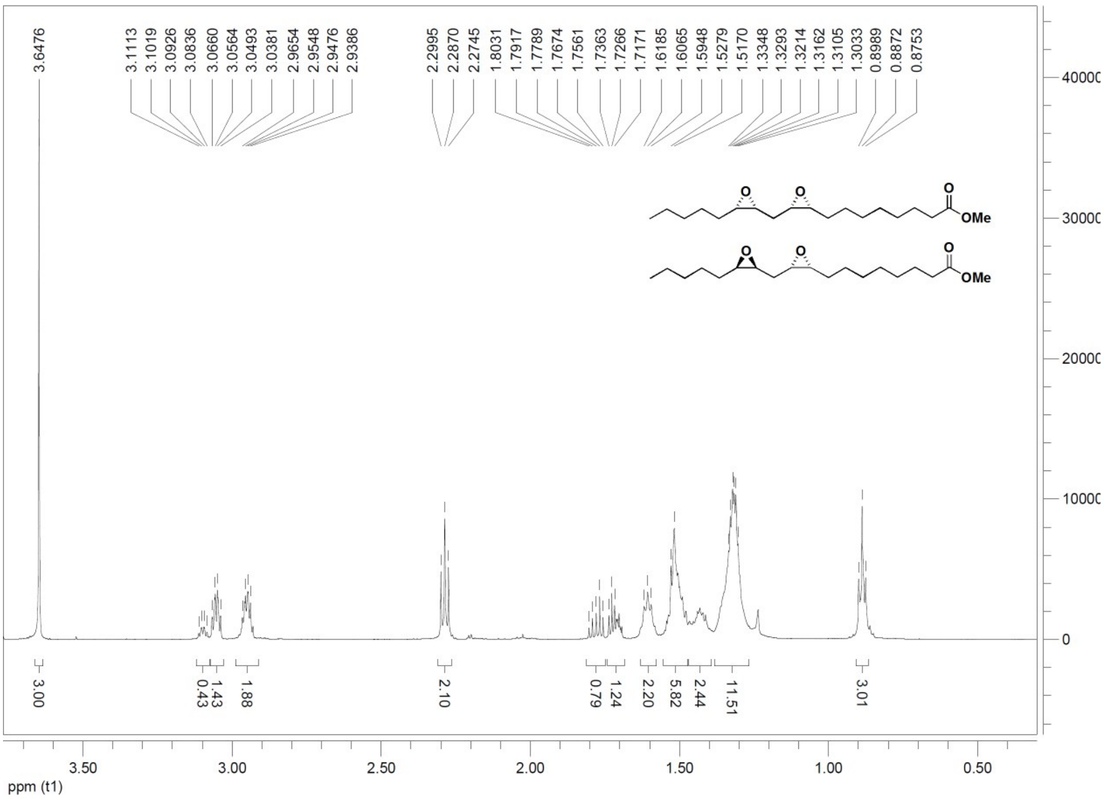
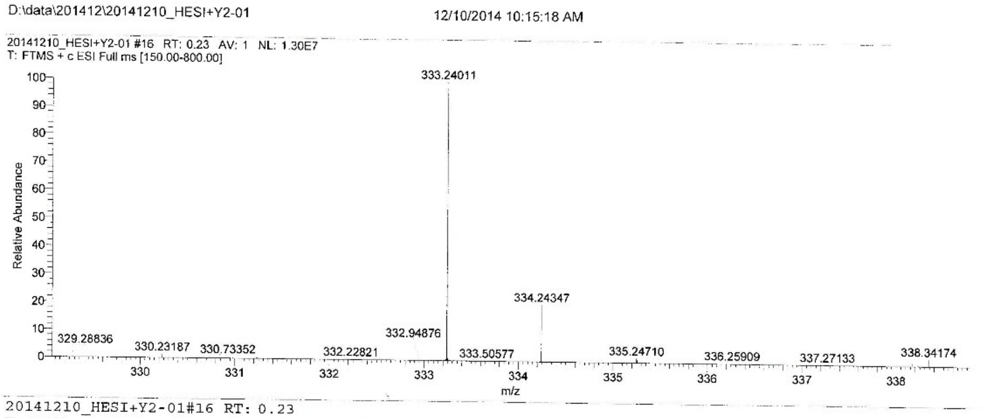


Fig. S8 ^{1}H-NMR spectra of 5 for the epoxidation of methyl linoleate

^{1}H-NMR (600MHz, $CDCl_3$): δ (ppm) = 3.65(s, -OCH_3), 2.96-3.09(m, -CH-O-CH-), 2.29(t, *J*=7.50Hz, -CH_2-CO-), 1.60(m, -CH2-CH-O-CH-CH2-CH-O-CH-CH2-), 1.31(m, -$(CH_2)_n$-) and 0.88(t, *J*=7.08Hz, -CH_3).



20141210_HESI+Y2-01#16 RT: 0.23
T: FTMS + c ESI Full ms [150.00-800.00]
m/z= 330.00000-340.00000

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
333.24011	12953338.0	100.00	333.24002	0.10	2.5	$C_{19}H_{34}O_3Na$
334.24347	2642665.3	20.40	334.24784	-4.37	2.0	$C_{19}H_{35}O_3Na$

Fig. S9 HRMS spectrum of 5 for the epoxidation of methyl linoleate

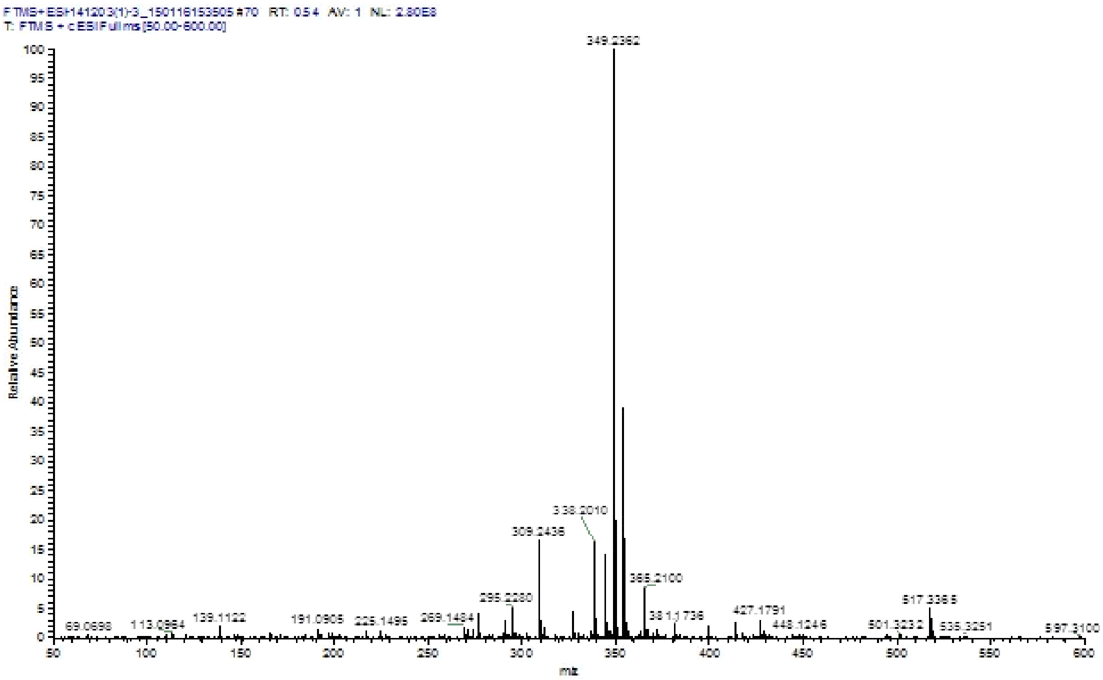


Fig. S10 HRMS spectrum of 6 for the epoxidation of methyl linoleate

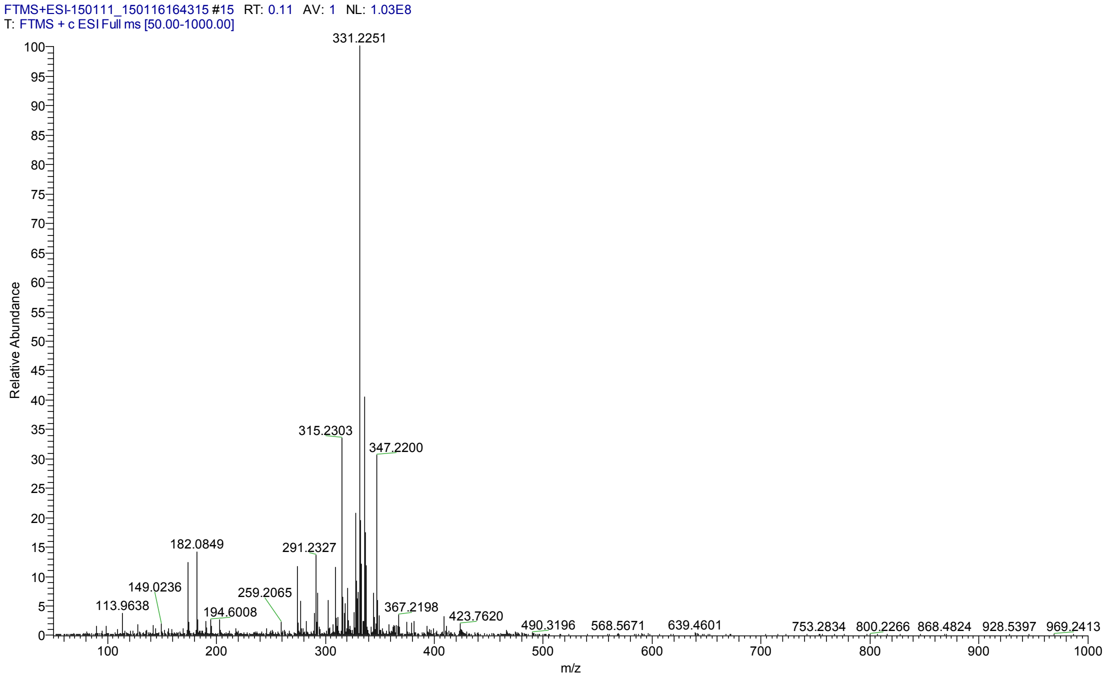


Fig. S11 HRMS spectrum for the epoxidation of methyl linolenate